

Xuhui Huang

List of Publications by Citations

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142
papers

7,857
citations

48
h-index

87
g-index

152
ext. papers

9,105
ext. citations

9.4
avg, IF

6.09
L-index

#	Paper	IF	Citations
142	Remdesivir, lopinavir, emetine, and homoharringtonine inhibit SARS-CoV-2 replication in vitro. <i>Antiviral Research</i> , 2020 , 178, 104786	10.8	528
141	Hydrophobic collapse in multidomain protein folding. <i>Science</i> , 2004 , 305, 1605-9	33.3	441
140	A tetraphenylethylene core-based 3D structure small molecular acceptor enabling efficient non-fullerene organic solar cells. <i>Advanced Materials</i> , 2015 , 27, 1015-20	24	334
139	Observation of a dewetting transition in the collapse of the melittin tetramer. <i>Nature</i> , 2005 , 437, 159-62	50.4	333
138	Why is the partial molar volume of CO ₂ so small when dissolved in a room temperature ionic liquid? Structure and dynamics of CO ₂ dissolved in [Bmim ⁺] [PF ₆ ⁻]. <i>Journal of the American Chemical Society</i> , 2005 , 127, 17842-51	16.4	307
137	What makes efficient circularly polarised luminescence in the condensed phase: aggregation-induced circular dichroism and light emission. <i>Chemical Science</i> , 2012 , 3, 2737	9.4	297
136	Monitoring and inhibition of insulin fibrillation by a small organic fluorogen with aggregation-induced emission characteristics. <i>Journal of the American Chemical Society</i> , 2012 , 134, 1680-9	16.4	293
135	Dewetting-induced collapse of hydrophobic particles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003 , 100, 11953-8	11.5	245
134	Massively parallel de novo protein design for targeted therapeutics. <i>Nature</i> , 2017 , 550, 74-79	50.4	235
133	Using generalized ensemble simulations and Markov state models to identify conformational states. <i>Methods</i> , 2009 , 49, 197-201	4.6	227
132	Structural basis of transcription: backtracked RNA polymerase II at 3.4 angstrom resolution. <i>Science</i> , 2009 , 324, 1203-6	33.3	195
131	Poly[(maleic anhydride)-alt-(vinyl acetate)]: A Pure Oxygenic Nonconjugated Macromolecule with Strong Light Emission and Solvatochromic Effect. <i>Macromolecules</i> , 2015 , 48, 64-71	5.5	183
130	A role for both conformational selection and induced fit in ligand binding by the LAO protein. <i>PLoS Computational Biology</i> , 2011 , 7, e1002054	5	172
129	Reduced Intramolecular Twisting Improves the Performance of 3D Molecular Acceptors in Non-Fullerene Organic Solar Cells. <i>Advanced Materials</i> , 2016 , 28, 8546-8551	24	143
128	Why Do Simple Molecules with "Isolated" Phenyl Rings Emit Visible Light?. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16264-16272	16.4	130
127	Blockade of EphA4 signaling ameliorates hippocampal synaptic dysfunctions in mouse models of Alzheimer's disease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 9959-64	11.5	127
126	Dynamics of an intrinsically disordered protein reveal metastable conformations that potentially seed aggregation. <i>Journal of the American Chemical Society</i> , 2013 , 135, 16092-101	16.4	125

125	Dramatic Differences in Aggregation-Induced Emission and Supramolecular Polymerizability of Tetraphenylethene-Based Stereoisomers. <i>Journal of the American Chemical Society</i> , 2017 , 139, 10150-10156	16.4	121
124	Rapid equilibrium sampling initiated from nonequilibrium data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 19765-9	11.5	115
123	X-ray structure and mechanism of RNA polymerase II stalled at an antineoplastic monofunctional platinum-DNA adduct. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 9584-9	11.5	105
122	Replica exchange with solute tempering: efficiency in large scale systems. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 5405-10	3.4	95
121	Dynamics of pyrophosphate ion release and its coupled trigger loop motion from closed to open state in RNA polymerase II. <i>Journal of the American Chemical Society</i> , 2012 , 134, 2399-406	16.4	94
120	AIEgen-based theranostic system: targeted imaging of cancer cells and adjuvant amplification of antitumor efficacy of paclitaxel. <i>Chemical Science</i> , 2017 , 8, 2191-2198	9.4	91
119	Millisecond dynamics of RNA polymerase II translocation at atomic resolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 7665-70	11.5	90
118	Dynamics of water confined in the interdomain region of a multidomain protein. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3704-11	3.4	88
117	Multifunctional AIEgens: Ready Synthesis, Tunable Emission, Mechanochromism, Mitochondrial, and Bacterial Imaging. <i>Advanced Functional Materials</i> , 2018 , 28, 1704589	15.6	84
116	Structural insight into RNA hairpin folding intermediates. <i>Journal of the American Chemical Society</i> , 2008 , 130, 9676-8	16.4	83
115	Topological methods for exploring low-density states in biomolecular folding pathways. <i>Journal of Chemical Physics</i> , 2009 , 130, 144115	3.9	82
114	Non-aromatic annulene-based aggregation-induced emission system via aromaticity reversal process. <i>Nature Communications</i> , 2019 , 10, 2952	17.4	79
113	Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. <i>Nanoscale</i> , 2016 , 8, 15173-80	7.7	77
112	Molecular dynamics study of the temperature-dependent Optical Kerr effect spectra and intermolecular dynamics of room temperature ionic liquid 1-methoxyethylpyridinium dicyanoamide. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 7837-49	3.4	77
111	White-Light Emission of a Binary Light-Harvesting Platform Based on an Amphiphilic Organic Cage. <i>Chemistry of Materials</i> , 2018 , 30, 1285-1290	9.6	77
110	Nanoscale dewetting transition in protein complex folding. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 9069-77	3.4	72
109	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 19018-22	3.4	71
108	Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation. <i>Rna</i> , 2011 , 17, 1066-75	5.8	67

107	Allosteric Effector ppGpp Potentiates the Inhibition of Transcript Initiation by DksA. <i>Molecular Cell</i> , 2018 , 69, 828-839.e5	17.6	66
106	Drying and hydrophobic collapse of paraffin plates. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 3546-52	3.4	65
105	The predicted structure of the headpiece of the Huntingtin protein and its implications on Huntingtin aggregation. <i>Journal of Molecular Biology</i> , 2009 , 388, 919-27	6.5	62
104	Stapling of unprotected helical peptides photo-induced intramolecular thiol-yne hydrothiolation. <i>Chemical Science</i> , 2016 , 7, 3325-3330	9.4	61
103	Dewetting transitions in protein cavities. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 1856-69	6.9	60
102	Simulating the T-jump-triggered unfolding dynamics of trpzip2 peptide and its time-resolved IR and two-dimensional IR signals using the Markov state model approach. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 5415-24	3.4	59
101	DNA-Encoded Dynamic Chemical Library and Its Applications in Ligand Discovery. <i>Journal of the American Chemical Society</i> , 2018 , 140, 15859-15867	16.4	59
100	Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. <i>Journal of Chemical Physics</i> , 2008 , 128, 205106	3.9	56
99	Quantitatively characterizing the ligand binding mechanisms of choline binding protein using Markov state model analysis. <i>PLoS Computational Biology</i> , 2014 , 10, e1003767	5	55
98	Bridge helix bending promotes RNA polymerase II backtracking through a critical and conserved threonine residue. <i>Nature Communications</i> , 2016 , 7, 11244	17.4	54
97	Synthesis, optical properties, and helical self-assembly of a bivaline-containing tetraphenylethene. <i>Scientific Reports</i> , 2016 , 6, 19277	4.9	53
96	RNA polymerase II trigger loop residues stabilize and position the incoming nucleotide triphosphate in transcription. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 15745-50	11.5	53
95	Constructing Markov State Models to elucidate the functional conformational changes of complex biomolecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018 , 8, e1343	7.9	49
94	Initiation complex structure and promoter proofreading. <i>Science</i> , 2011 , 333, 633-7	33.3	48
93	Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. <i>Nature Communications</i> , 2017 , 8, 15639	17.4	47
92	Quantitative comparison of alternative methods for coarse-graining biological networks. <i>Journal of Chemical Physics</i> , 2013 , 139, 121905	3.9	42
91	Network models for molecular kinetics and their initial applications to human health. <i>Cell Research</i> , 2010 , 20, 622-30	24.7	41
90	Force field development for cofactors in the photosystem II. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1969-80	3.5	40

89	A two-state model for the dynamics of the pyrophosphate ion release in bacterial RNA polymerase. <i>PLoS Computational Biology</i> , 2013 , 9, e1003020	5	40
88	Markov State Models Reveal a Two-Step Mechanism of miRNA Loading into the Human Argonaute Protein: Selective Binding followed by Structural Re-arrangement. <i>PLoS Computational Biology</i> , 2015 , 11, e1004404	5	39
87	Hierarchical Nystroth methods for constructing Markov state models for conformational dynamics. <i>Journal of Chemical Physics</i> , 2013 , 138, 174106	3.9	37
86	The influence of spacer units on molecular properties and solar cell performance of non-fullerene acceptors. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 20108-20112	13	36
85	Dynamic protein conformations preferentially drive energy transfer along the active chain of the photosystem II reaction centre. <i>Nature Communications</i> , 2014 , 5, 4170	17.4	33
84	Constructing multi-resolution Markov State Models (MSMs) to elucidate RNA hairpin folding mechanisms. <i>Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing</i> , 2010 , 228-39	1.3	33
83	Unique Roles of the Non-identical MCM Subunits in DNA Replication Licensing. <i>Molecular Cell</i> , 2017 , 67, 168-179	17.6	31
82	Elucidation of the Dynamics of Transcription Elongation by RNA Polymerase II using Kinetic Network Models. <i>Accounts of Chemical Research</i> , 2016 , 49, 687-94	24.3	30
81	Automatic state partitioning for multibody systems (APM): an efficient algorithm for constructing Markov state models to elucidate conformational dynamics of multibody systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 17-27	6.4	29
80	Achieving enhanced cell penetration of short conformationally constrained peptides through amphiphilicity tuning. <i>Chemical Science</i> , 2017 , 8, 7576-7581	9.4	29
79	Synaptic Targeting and Function of SAPAPs Mediated by Phosphorylation-Dependent Binding to PSD-95 MAGUKs. <i>Cell Reports</i> , 2017 , 21, 3781-3793	10.6	29
78	Specific and Quantitative Detection of Albumin in Biological Fluids by Tetrazolate-Functionalized Water-Soluble AIEgens. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 29619-29629	9.5	26
77	Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 13990-13994	16.4	26
76	A deep learning framework to predict binding preference of RNA constituents on protein surface. <i>Nature Communications</i> , 2019 , 10, 4941	17.4	25
75	A fast parallel clustering algorithm for molecular simulation trajectories. <i>Journal of Computational Chemistry</i> , 2013 , 34, 95-104	3.5	25
74	Multiscale modeling of macromolecular biosystems. <i>Briefings in Bioinformatics</i> , 2012 , 13, 395-405	13.4	23
73	Application of Markov State Models to simulate long timescale dynamics of biological macromolecules. <i>Advances in Experimental Medicine and Biology</i> , 2014 , 805, 29-66	3.6	22
72	Adaptive partitioning by local density-peaks: An efficient density-based clustering algorithm for analyzing molecular dynamics trajectories. <i>Journal of Computational Chemistry</i> , 2017 , 38, 152-160	3.5	21

71	Single-Molecule Investigations of Conformation Adaptation of Porphyrins on Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1241-1247	6.4	17
70	A Flexible Domain-Domain Hinge Promotes an Induced-fit Dominant Mechanism for the Loading of Guide-DNA into Argonaute Protein in <i>Thermus thermophilus</i> . <i>Journal of Physical Chemistry B</i> , 2016 , 120, 2709-20	3.4	17
69	Crystallographic Snapshots of Class A β -Lactamase Catalysis Reveal Structural Changes That Facilitate β -Lactam Hydrolysis. <i>Journal of Biological Chemistry</i> , 2017 , 292, 4022-4033	5.4	16
68	Ca-Induced Rigidity Change of the Myosin VIIa IQ Motif-Single β -Helix Lever Arm Extension. <i>Structure</i> , 2017 , 25, 579-591.e4	5.2	15
67	Kinetics-Controlled Amphiphile Self-Assembly Processes. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1798-1803	6.4	14
66	Elucidation of the conformational dynamics of multi-body systems by construction of Markov state models. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 30228-30235	3.6	14
65	Clustering algorithms to analyze molecular dynamics simulation trajectories for complex chemical and biological systems. <i>Chinese Journal of Chemical Physics</i> , 2018 , 31, 404-420	0.9	14
64	Aggregation-Induced-Emission-Active Macrocycle Exhibiting Analogous Triply and Singly Twisted M β ius Topologies. <i>Chemistry - A European Journal</i> , 2015 , 21, 11707-11	4.8	13
63	Mechanism of action of thalassospiramides, a new class of calpain inhibitors. <i>Scientific Reports</i> , 2015 , 5, 8783	4.9	13
62	1'-Ribose cyano substitution allows Remdesivir to effectively inhibit nucleotide addition and proofreading during SARS-CoV-2 viral RNA replication. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 5852-5863	3.6	13
61	Impact of template backbone heterogeneity on RNA polymerase II transcription. <i>Nucleic Acids Research</i> , 2015 , 43, 2232-41	20.1	12
60	Identification of new EphA4 inhibitors by virtual screening of FDA-approved drugs. <i>Scientific Reports</i> , 2018 , 8, 7377	4.9	12
59	Dynamics of the conformational transitions during the dimerization of an intrinsically disordered peptide: a case study on the human islet amyloid polypeptide fragment. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 29892-29904	3.6	12
58	Molecular mechanisms of RNA polymerase II transcription elongation elucidated by kinetic network models. <i>Current Opinion in Structural Biology</i> , 2018 , 49, 54-62	8.1	11
57	Controlling the Integration of Polyvinylpyrrolidone onto Substrate by Quartz Crystal Microbalance with Dissipation To Achieve Excellent Protein Resistance and Detoxification. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 18684-92	9.5	11
56	Elucidating dominant pathways of the nano-particle self-assembly process. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 23494-9	3.6	11
55	Constructing kinetic models to elucidate structural dynamics of a complete RNA polymerase II elongation cycle. <i>Physical Biology</i> , 2014 , 12, 016004	3	10
54	Investigating the structural origin of trpzip2 temperature dependent unfolding fluorescence line shape based on a Markov state model simulation. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 12669-76	3.4	10

53	Two symmetric arginine residues play distinct roles in Argonaute DNA guide strand-mediated DNA target cleavage. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 845-853	11.5	10
52	Mechanistic Insights and Rational Design of a Versatile Surface with Cells/Bacteria Recognition Capability via Orientated Fusion Peptides. <i>Advanced Science</i> , 2019 , 6, 1801827	13.6	9
51	Structural Model of RNA Polymerase II Elongation Complex with Complete Transcription Bubble Reveals NTP Entry Routes. <i>PLoS Computational Biology</i> , 2015 , 11, e1004354	5	9
50	Target search and recognition mechanisms of glycosylase AlkD revealed by scanning FRET-FCS and Markov state models. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 21889-21895	11.5	9
49	Structural dissection of an interaction between transcription initiation and termination factors implicated in promoter-terminator cross-talk. <i>Journal of Biological Chemistry</i> , 2018 , 293, 1651-1665	5.4	9
48	A theoretical study on the dynamics of light harvesting in the dimeric photosystem II core complex: regulation and robustness of energy transfer pathways. <i>Faraday Discussions</i> , 2019 , 216, 94-115	3.6	8
47	TAPS: A traveling-salesman based automated path searching method for functional conformational changes of biological macromolecules. <i>Journal of Chemical Physics</i> , 2019 , 150, 124105	3.9	8
46	Intrinsic Cleavage of RNA Polymerase II Adopts a Nucleobase-independent Mechanism Assisted by Transcript Phosphate. <i>Nature Catalysis</i> , 2019 , 2, 228-235	36.5	8
45	Organic Solar Cells: A Tetraphenylethylene Core-Based 3D Structure Small Molecular Acceptor Enabling Efficient Non-Fullerene Organic Solar Cells (Adv. Mater. 6/2015). <i>Advanced Materials</i> , 2015 , 27, 1014-1014	24	8
44	Strand-specific (asymmetric) contribution of phosphodiester linkages on RNA polymerase II transcriptional efficiency and fidelity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, E3269-76	11.5	8
43	An efficient Bayesian kinetic lumping algorithm to identify metastable conformational states via Gibbs sampling. <i>Journal of Chemical Physics</i> , 2018 , 149, 072337	3.9	8
42	Maltose-binding protein effectively stabilizes the partially closed conformation of the ATP-binding cassette transporter MalFGK. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 9366-9373	3.6	7
41	On the advantages of exploiting memory in Markov state models for biomolecular dynamics. <i>Journal of Chemical Physics</i> , 2020 , 153, 014105	3.9	7
40	Understanding the core of RNA interference: The dynamic aspects of Argonaute-mediated processes. <i>Progress in Biophysics and Molecular Biology</i> , 2017 , 128, 39-46	4.7	7
39	Role of bacterial RNA polymerase gate opening dynamics in DNA loading and antibiotics inhibition elucidated by quasi-Markov State Model. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	7
38	Elucidating molecular mechanisms of functional conformational changes of proteins via Markov state models. <i>Current Opinion in Structural Biology</i> , 2021 , 67, 69-77	8.1	7
37	Reference interaction site model with hydrophobicity induced density inhomogeneity: An analytical theory to compute solvation properties of large hydrophobic solutes in the mixture of polyatomic solvent molecules. <i>Journal of Chemical Physics</i> , 2015 , 143, 054110	3.9	6
36	The hydrolytic water molecule of Class A β -lactamase relies on the acyl-enzyme intermediate ES* for proper coordination and catalysis. <i>Scientific Reports</i> , 2020 , 10, 10205	4.9	6

35	Harnessing complexity in molecular self-assembly using computer simulations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 6767-6776	3.6	6
34	Role of 1ERibose Cyano Substitution for Remdesivir to Effectively Inhibit Nucleotide Addition and Proofreading in SARS-CoV-2 Viral RNA Replication		6
33	Path lumping: An efficient algorithm to identify metastable path channels for conformational dynamics of multi-body systems. <i>Journal of Chemical Physics</i> , 2017 , 147, 044112	3.9	5
32	Transcriptional processing of an unnatural base pair by eukaryotic RNA polymerase II. <i>Nature Chemical Biology</i> , 2021 , 17, 906-914	11.7	5
31	Recent Developments in Integral Equation Theory for Solvation to Treat Density Inhomogeneity at Solute-Solvent Interface. <i>Advanced Theory and Simulations</i> , 2019 , 2, 1900049	3.5	4
30	Functional interplay between NTP leaving group and base pair recognition during RNA polymerase II nucleotide incorporation revealed by methylene substitution. <i>Nucleic Acids Research</i> , 2016 , 44, 3820-8	20.1	4
29	Bridging the Gap Between Optical Spectroscopic Experiments and Computer Simulations for Fast Protein Folding Dynamics. <i>Current Physical Chemistry</i> , 2012 , 2, 45-58	0.5	4
28	THEORETICAL INVESTIGATIONS ON ELUCIDATING FUNDAMENTAL MECHANISMS OF CATALYSIS AND DYNAMICS INVOLVED IN TRANSCRIPTION BY RNA POLYMERASE. <i>Journal of Theoretical and Computational Chemistry</i> , 2013 , 12, 1341005	1.8	4
27	DATA-DRIVEN TIGHT FRAME FOR CRYO-EM IMAGE DENOISING AND CONFORMATIONAL CLASSIFICATION 2018 ,		4
26	Markov State Models to Study the Functional Dynamics of Proteins in the Wake of Machine Learning. <i>Jacs Au</i> , 2021 , 1, 1330-1341		4
25	Molecular basis defining the selectivity of substituted isoquinolinones for the melatonin MT receptor. <i>Biochemical Pharmacology</i> , 2020 , 177, 114020	6	3
24	Understanding molecular recognition by kinetic network models constructed from molecular dynamics simulations. <i>Advances in Experimental Medicine and Biology</i> , 2014 , 797, 107-14	3.6	3
23	Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. <i>Angewandte Chemie</i> , 2016 , 128, 14196-14200	3.6	3
22	Constructing Kinetic Network Models to Elucidate Mechanisms of Functional Conformational Changes of Enzymes and Their Recognition with Ligands. <i>Methods in Enzymology</i> , 2016 , 578, 343-71	1.7	3
21	Incorporation efficiency and inhibition mechanism of 2'-substituted nucleotide analogs against SARS-CoV-2 RNA-dependent RNA polymerase. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 20117-20128	3.6	3
20	Construction of diverse peptide structural architectures chemoselective peptide ligation. <i>Chemical Science</i> , 2021 , 12, 7091-7097	9.4	3
19	Microsecond timescale MD simulations at the transition state of HMGR predict remote allosteric residues. <i>Chemical Science</i> , 2021 , 12, 6413-6418	9.4	3
18	8-Oxo-guanine DNA damage induces transcription errors by escaping two distinct fidelity control checkpoints of RNA polymerase II. <i>Journal of Biological Chemistry</i> , 2019 , 294, 4924-4933	5.4	2

17	Three-site and five-site fixed-charge water models compatible with AMOEBA force field. <i>Journal of Computational Chemistry</i> , 2020 , 41, 1034-1044	3.5	2
16	Identifying Transcription Error-Enriched Genomic Loci Using Nuclear Run-on Circular-Sequencing Coupled with Background Error Modeling. <i>Journal of Molecular Biology</i> , 2020 , 432, 3933-3949	6.5	2
15	3DRISM-HI-D2MSA: an improved analytic theory to compute solvent structure around hydrophobic solutes with proper treatment of solute-solvent electrostatic interactions. <i>Molecular Physics</i> , 2018 , 116, 1003-1013	1.7	2
14	Adaptive Seeding: A New Method for Simulating Biologically Relevant Timescales. <i>Biophysical Journal</i> , 2009 , 96, 575a	2.9	2
13	Critical role of backbone coordination in the mRNA recognition by RNA induced silencing complex. <i>Communications Biology</i> , 2021 , 4, 1345	6.7	2
12	Are endoplasmic reticulum subdomains shaped by asymmetric distribution of phospholipids? Evidence from a <i>C. elegans</i> model system. <i>BioEssays</i> , 2021 , 43, e2000199	4.1	2
11	Entropy of stapled peptide inhibitors in free state is the major contributor to the improvement of binding affinity with the GK domain. <i>RSC Chemical Biology</i> , 2021 , 2, 1274-1284	3	2
10	A novel mechanism of enhanced transcription activity and fidelity for influenza A viral RNA-dependent RNA polymerase. <i>Nucleic Acids Research</i> , 2021 , 49, 8796-8810	20.1	2
9	Temperature-dependent kinetic pathways of heterogeneous ice nucleation competing between classical and non-classical nucleation. <i>Nature Communications</i> , 2021 , 12, 4954	17.4	2
8	Elucidation of the key role of Pt-Pt interactions in the directional self-assembly of platinum(II) complexes.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022 , 119, e2116543119	11.5	2
7	Improving the productivity of monodisperse polyhedral cages by the rational design of kinetic self-assembly pathways. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10030-10037	3.6	1
6	Enhancing pairwise state-transition weights: A new weighting scheme in simulated tempering that can minimize transition time between a pair of conformational states. <i>Journal of Chemical Physics</i> , 2016 , 144, 154107	3.9	1
5	Role of Surface Templating on Ice Nucleation Efficiency on a Silver Iodide Surface. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18857-18865	3.8	1
4	The mechanism of action of T-705 as a unique delayed chain terminator on influenza viral polymerase transcription. <i>Biophysical Chemistry</i> , 2021 , 277, 106652	3.5	1
3	Elucidating Mechanisms of Molecular Recognition Between Human Argonaute and miRNA Using Computational Approaches. <i>Methods in Molecular Biology</i> , 2017 , 1517, 251-275	1.4	
2	Mechanochromism: Multifunctional AIEgens: Ready Synthesis, Tunable Emission, Mechanochromism, Mitochondrial, and Bacterial Imaging (Adv. Funct. Mater. 1/2018). <i>Advanced Functional Materials</i> , 2018 , 28, 1870006	15.6	
1	A comprehensive mechanism for 5-carboxylcytosine-induced transcriptional pausing revealed by Markov state models. <i>Journal of Biological Chemistry</i> , 2021 , 296, 100735	5.4	